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New modeling strategies for the computational characterization of nanobioparticles

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Nanobiotechnology is a field of science focused on the design, synthesis, characterization and application of materials and devices on the nanoscale to biological problems. The success of this promising area of research hinges in our ability to characterize, and eventually predict and control, the properties of nanoscale particles and their behavior in realistic biological environments. Particles of this size behave in ways that are intrinsically different than those at meso and sub-nano scale. Therefore, the characterization of nanoparticles by computational means requires the definition of new microscopic criteria to match the modeled parameters with macroscopically observed toxic effects or ADME parameters. In this work we will present our efforts at devising strategies that, from simulations of nanoparticles in simple environments, will allow the computation of properties related to their behavior in more complex environments. The approach presented departs from classical extensions of QSAR type calculations to nanoparticles, relying instead in a series of sensitivity analysis techniques that probe the stability of the particle properties with respect to a number of challenges. Particles will be suitable candidates for biological use only if the range of their sensitivity to those challenges is narrowly confined. The nature of the parameters explored and the use of this approach in general cases will be discussed by presenting our results using metal-loaded fullerenes, and extending it over our early efforts with gold particles and dendrimer simulations.

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